



chain nodes :

29 30 31 32 33 34 35 36 37 46 47 48 49 50 51 52 53 54 55 56 57

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26
27 28

chain bonds :

2-31 5-29 8-30 11-46 15-47 18-48 20-49 23-51 29-30 31-32 32-33 33-34 34-35 34-36
36-37 46-47 48-49 49-50 51-52 52-53 53-54 54-55 54-56 56-57

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 7-28 8-9 9-10 10-11 11-12 12-25 13-14 13-18
14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23 23-24 25-26 26-27 27-28

exact/norm bonds :

1-2 1-6 2-3 2-31 3-4 4-5 5-6 5-29 8-30 11-46 13-14 13-18 14-15 15-16 15-47 16-17
17-18 18-48 23-51 29-30 33-34 34-35 46-47 48-49 49-50 53-54 54-55

exact bonds :

20-49 31-32 32-33 34-36 36-37 51-52 52-53 54-56 56-57

normalized bonds :

7-8 7-12 7-28 8-9 9-10 10-11 11-12 12-25 19-20 19-24 20-21 21-22 22-23 23-24
25-26 26-27 27-28

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS 31:CLASS
32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 46:CLASS 47:CLASS 48:CLASS
49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS 54:CLASS 55:CLASS 56:CLASS 57:CLASS